

REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-01-

0353

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

ning
s for
e of

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE May 7, 2001	3. REPORT TYPE AND DATES COVERED Final, 3/15/98 - 3/14/01
4. TITLE AND SUBTITLE The Growth of Nanostructures and Composite Films on Solids: Simulation and Phenomelological Theory		5. FUNDING NUMBERS F49620-98-1-0366
6. AUTHOR(S) Dr. Horia Metiu		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Chemistry & Biochemistry University of California Santa Barbara, CA 93106		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NL 110 Duncan Avenue, Room B115 Bolling AFB, DC 20332-8050		10. SPONSORING/MONITORING AGENCY REPORT NUMBER
11. SUPPLEMENTARY NOTES		
12a. DISTRIBUTION/AVAILABILITY STATEMENT Distribution unlimited, approved for public release		AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFOSR) NOTICE OF TRANSMITTAL DTIC. THIS TECHNICAL REPORT HAS BEEN REVIEWED AND IS APPROVED FOR PUBLIC RELEASE LAW AFR 190-12. DISTRIBUTION IS UNLIMITED.
13. ABSTRACT (Maximum 200 words) We have studied how the morphology of films grown by epitaxy changes after deposition, if we change the temperature. We have determined by simulations how isolated islands on a solid surface move or shrink by evaporation. We developed new methods to study how an ensemble of islands evolves when heated or when strain is imposed on the surface. This work provides an understanding of basic phenomena taking place during epitaxy.		
14. SUBJECT TERMS nano-structures, composite films, phenomenological theory.		15. NUMBER OF PAGES 2
		16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED
20. LIMITATION OF ABSTRACT UL		

20010606 043

Final Report, Grant F 49620-98-1-0366 "The Growth of Nanostructures and Composite Films on Solids: Simulations and Phenomenological Theory"

The resources provided by this grant were used for theoretical research in several areas. We performed simulations of a number of phenomena taking place in the early stages of film growth by epitaxy. We have provided a complete description of how the islands formed on the surface during deposition, move[3], evaporate[9], and change shape[4]. We developed a method to simulate coarsening of these islands on a very long time and space scale[5,7]. We proposed and documented by simulations[8,10] that nucleation and growth can be controlled by imposing a periodic strain on the substrate, which will lead to the formation of a periodic array of islands of equal size. To achieve this kind of control has been one of the main goals of nano-science. It has been observed that islands grown on a surface prefer a specific size. We have shown[1] that this may happen because the island size fits a natural length of the electronic wave-function.

In the second part of the grant's duration, we switched to studying various catalytic systems. We have shown that surface strain modifies very substantially the adsorption isotherm[11] and this may explain why ultrasound passing through a catalyst changes its activity. Our current work examines the electronic properties of the γ -alumina[13] (which is the support of choice in most catalysts). This is the first calculation on this very demanding system. We have also determined how Pd atoms migrate on γ -alumina surface[14]. The adsorption of a metal on the surface of another metal, can modify its properties and we looked[16] at how the capacity of adsorbing CO is modified when Fe, Cu, or Ni islands are adsorbed on Ag. We were prompted to do this by very elegant single-molecule experiments by Wilson Ho, whose conclusions are confirmed by our calculations. Finally, we developed a new method for deriving potential expressions from *ab initio* energy calculations[2], proposed a new numerical method for performing quantum dynamics[15], developed an algorithm for solving Maxwell equations and used it to examine how the electromagnetic field under an STM tip is enhanced[12], and wrote a review article of our work on rate theory in quantum systems.

References

1. K-J. Jin, G. D. Mahan, H. Metiu, and Z. Zhang, *Phys. Rev. Lett.* **80**, 1026-1027 (1998)
2. D. E. Makarov and H. Metiu, *J. Chem. Phys.* **108**, 590-598 (1998)
3. A. Bogicevic, S. Liu, J. Jacobsen, B. Lundqvist, and H. Metiu, *Phys. Rev. B* **57**, R9459-R9462 (1998)
4. S. Liu and H. Metiu, *Surface Sci.* **405**, L497-L502 (1998)
5. H. Metiu, T. R. Mattsson, and G. Mills, in *Mechanisms and Principles of Epitaxial Growth in Metallic Systems*, L. T. Wille, C. P. Burmester, K. Terakura, and G. Comsa, eds., Materials Research Society Proc. **528** (1998), pp. 133-143
6. H. Metiu, in *Classical and Quantum Dynamics in Condensed Phase Simulations*, B. J. Berne, G. Ciccoti, and D. F. Coker, Editors, World Scientific (1998), pp. 781-803
7. T. R. Mattsson, G. Mills, and H. Metiu, *J. Chem. Phys.* **110**, 12 151-12 160 (1999)
8. T. R. Mattsson and H. Metiu, *Appl. Phys. Lett.* **75**, 926-928 (1999)
9. G. Mills, T. R. Mattsson, L. Møllnitz, and H. Metiu, *J. Chem. Phys.* **111**, 8639 (1999)
10. T. R. Mattsson and H. Metiu, *J. Chem. Phys.* **113**, 10323-10332 (2000)
11. M. W. Wu and H. Metiu, *J. Chem. Phys.* **113**, 1177-1183 (2000)
12. R. E. Larsen and H. Metiu, *J. Chem. Phys.*, scheduled for March 22, 2001, issue
13. Vacancy distributions in bulk and at the (001) surface of γ -alumina, A. Vijay, G. Mills and H. Metiu, in preparation
14. The mobility of Pd atoms on the (001) surface of γ -alumina, A. Vijay, G. Mills and H. Metiu, in preparation
15. A new method for computing the time propagator, the Green function and the spectral density operators in quantum dynamics, in preparation
16. CO adsorption on small Fe, Cu, and Ni islands supported on Ag(110), G. Mills and H. Metiu, in preparation